U.S. EPA Environmental Response Team
Trace Atmospheric Gas Analyzer (TAGA) 6000E
Mass Spectrometer/Mass Spectrometer (MS/MS)

The Trace Atmospheric Gas Analyzer (TAGA) 6000E mass spectrometer/mass spectrometer (MS/MS) is a real-time, direct-air sampling, laboratory instrument which is mounted in a vehicle. The TAGA has demonstrated the following analytical capabilities:

- Direct-air sampling and analysis of organic compounds in the ambient air at the part-per-billion by volume (ppbv) level while mobile monitoring along roads in an effort to detect fugitive emissions originating from suspected sources. This technique has been used to 1) isolate contributions of upwind sources from the downwind matrix; 2) locate the plume's centerline concentrations so additional sampling and analysis techniques (i.e., Summa canisters and gas chromatography /mass spectrometry (GC/MS)) can confirm results; and 3) model the plume capture to predict source emission rates.

- Direct-air sampling and analysis of organic compounds in the indoor air of houses and buildings adjacent to Superfund sites to determine whether contaminants are migrating from the adjacent site into the structures. This technique monitors, in real time, the indoor air levels and determines the potential entry locations using a Teflon sampling hose.

- Rapid analysis of soil gas samples collected in Tedlar bags in order to support extent of contamination studies conducted at or near underground sources of volatile organic compounds. This technique provides rapid analysis of the Tedlar bags, which reduces the error associated with holding times in the bags. It also allows better utilization of resources during the investigation.

- Rapid analysis of gas samples collected in Tedlar bags in order to support engineering feasibility studies. This technique provides rapid analysis of the Tedlar bags, which allows operating parameters to be changed while examining the emissions as a function of time for the variable changed.

- Mass spectral information for materials collected in vials. This technique gives information that can assist in determining the molecular structure and/or the identity of volatile organic compounds.

- Direct-air sampling and analysis of organic compounds in the ambient air at industrial settings. This technique provides information concerning the location, identity, and quantity of the emissions to assist in the enforcement of local, state, and federal codes.

The general theory of the TAGA 6000E MS/MS utilizes the technique of triple quadrupole MS/MS to differentiate and quantitate compounds. The analysis procedure involves multiple sequential steps. The initial step in the MS/MS process involves simultaneous chemical ionization of the compounds present in a sample of ambient air. The ionization produces either positive or negative ions by donating or removing one or more electrons. The chemical ionization is a "soft" ionization technique which allows ions to be formed with little or no structural fragmentation. These ions are called parent ions.

The parent ions with different mass-to-charge (m/z) ratios are separated by the first quadrupole (the first MS of the MS/MS system). The quadrupole scans selected m/z ratios allowing only the parent ions with these ratios to pass through the quadrupole. Parent ions with m/z ratios different from those selected are discriminated electronically and fail to pass through the quadrupole.

The parent ions selected in the first quadrupole are accelerated through a cloud of uncharged argon atoms which are introduced normal to the ion path in the second quadrupole. A portion of the parent ions entering the second quadrupole fragment as they collide with the argon atoms. These fragmented ions are called daughter ions. This process, in the second quadrupole, is called collision induced dissociation (CID).

The daughter ions are separated according to their m/z ratios by the third quadrupole (the second MS of the MS/MS system). The quadrupole scans selected m/z ratios allowing only the daughter ions with these ratios to pass through the quadrupole. Daughter ions with m/z ratios different from those selected are discriminated electronically and fail to pass through the quadrupole. Daughter ions with the selected m/z ratios are then counted by an electron multiplier. The resulting signals are measured in ion counts per second (ICPS) for each parent/daughter ion pair selected. The intensity of the ICPS for each parent/daughter ion pair is directly proportional to the ambient air concentration of the organic compound that produced the ion pair.

If the ions are singly charged, the m/z ratios of the ions are equal to the ion masses (atomic mass units). Therefore, the terms parent and daughter masses are synonymous with parent and daughter ion m/z ratios.

The TAGA can perform mobile, ambient air monitoring using a direct-air sampling system along roads adjacent to suspected sources to detect emissions originating from these locations. Outside ambient air is continuously drawn through a port in the wall of the TAGA bus at a flow rate of approximately one and one-half liters per second. The air then passes through a glass splitter where the pressure gradient between the mass spectrometer core and the atmosphere causes a sample flow of approximately 10 milliliters per minute into the ionization source through a heated transfer line. The flow into the low pressure chemical ionization (LPCI) source is manually controlled and adjusted so that the ionization source pressure is maintained at an optimum value, which is about one torr. The remaining air flow is drawn through the air motor and vented from the bus.

The TAGA can perform mobile monitoring in the parent ion or parent/daughter ion pair monitoring mode. As the mobile monitoring proceeds, the operator presses the letter keys (flags) sequentially to denote events or locations during the monitoring. This information is also recorded on the operator's log sheet. The intensity of each parent ion or parent/daughter ion pair monitored by the TAGA is recorded by the Plessey computer in a file on the hard disk. One set of measurements for each ion is called a sequence.

The TAGA can perform stationary, ambient air monitoring with or without the Teflon hose. Without the Teflon hose, the monitoring is conducted identically to the mobile monitoring except that the bus is not in motion. With the Teflon hose, one end is connected to the sampling port on the TAGA bus and the distal end is moved to an area of concern and the sample is transported to the TAGA through the Teflon hose. This technique allows one to analyze, in real time, areas that are not physically accessible to the bus for mobile monitoring.

The TAGA can analyze Tedlar bag samples by directly connecting the sample bag to the heated transfer line of the TAGA and allowing the sample to be drawn directly into the source. This technique allows one to analyze a discreet sample from areas that are not physically accessible to the bus or the Teflon hose.